A Computer Generated Reduced Iso-Octane Chemical Kinetic Mechanism Applied to Simulation of HCCI Combustion

S.M. Aceves, J. Martinez-Frias, D. Flowers, J.R. Smith
R. Dibble, J.Y. Chen

U.S. Department of Energy

Lawrence
Livermore
National
Laboratory

August 12, 2002

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Salvador M. Aceves, Joel Martinez-Frias, Daniel Flowers, J. Ray Smith
Lawrence Livermore National Laboratory

Robert Dibble, J.Y. Chen
University of California Berkeley

ABSTRACT

This paper shows how a computer can systematically remove non-essential chemical reactions from a large chemical kinetic mechanism. The computer removes the reactions based upon a single solution using a detailed mechanism. The resulting reduced chemical mechanism produces similar numerical predictions significantly faster than predictions that use the detailed mechanism.

Specifically, a reduced chemical kinetics mechanism for iso-octane has been derived from a detailed mechanism by eliminating unimportant reaction steps and species. The reduced mechanism has been developed for the specific purpose of fast and accurate prediction of ignition timing in an HCCI engine. The reduced mechanism contains 199 species and 383 reactions, while the detailed mechanism contains 859 species and 3606 reactions. Both mechanisms have been used in numerical simulation of HCCI combustion. The simulations show that the reduced mechanism predicts pressure traces and heat release with good accuracy, similar to the accuracy obtained with the detailed mechanism.

As may be expected, emissions of hydrocarbon and carbon monoxide are not as well predicted with the reduced mechanism as with the detailed mechanism, since the reduced mechanism was targeted for predicting HCCI ignition and not HC and CO emissions. Considering that the reduced mechanism requires about 25 times less computational time than the detailed mechanism (2 hours vs. 2 days), the ability to automatically generate a problem specific reduced mechanism is an important new tool for combustion research in general.

INTRODUCTION

It is generally believed that a complete chemical mechanism, combined with the Navier Stokes equations will lead to numerical simulations of **all** combustion phenomena. This includes flame speeds as a function of temperature, pressure and stoichiometry; chemiluminescence from flames; explosion limits; pollutant formation in flames; flammability limits at all temperatures and pressures; and all other features. In practice, a numerical simulation that carries complete physics will likely tax the speed of any computer; this is certainly true if the flow is turbulent. Such a complete description is seldom attempted. Out of necessity, one makes judicious assumptions that reduce the dimensionality of the problem, in both fluid dynamic space and-or in chemical kinetic space, until a tractable problem is achieved. A reduction in dimensionality of chemical kinetic space means removal of "unimportant" species. This reduction is done at some loss in fidelity, yet, chemical kinetic mechanisms can be judiciously "reduced." Such reduced mechanisms can reduce the computational time while retaining key important features and losing features that are deemed unimportant. Thus, autoignition chemistry can be retained while other details, such as soot production chemistry, for example, may not be retained in the "simplified" ignition mechanism.

In the past, a reduced chemical kinetic mechanism was the result of trial and error. Recent developments in understanding chemical kinetics by computer methods, such as Computational Singular Perturbation (CSP) [1] and Intrinsic Low Dimensional Manifold (ILDM) [2], allow systematic identification unimportant species and reaction steps. Reviews on methods for mechanism reduction and on reduced chemistry have been provided by Frenchlack [3] and Griffiths [4]. Specific applications to HCCI chemical kinetics using automatic approaches have been illustrated recently for natural gas combustion [5,6]. This paper reports the development of a reduced chemical kinetic mechanism for oxidation of iso-octane from a large mechanism using a computer with an automatic procedure. We then insert the reduced mechanism, of iso-octane oxidation, into a numerical simulation of HCCI combustion.

The need for a reduced mechanism is illustrated by a brief review of our previous work on simulation of HCCI engines. We have combined detailed chemical kinetics with fluid mechanics for high fidelity predictions of combustion in HCCI engines. These early successes were done with relatively simple fuels (methane, propane) that have relatively small detailed chemical kinetic mechanisms. With these simple fuels, computational times were about 2 hours, and we had little need for reduced mechanisms. As we evolved to simulations of HCCI using more complicated fuels, our numerical predictions were taking more and more computational time; the run time increasing as the square of the number of species. These long-computational-time simulations, using the detailed chemical mechanisms, predict many parameters well, such as ignition timing, pressure trace, and emissions of pollutants. However, such long computational times are impractical for surveys and optimization studies. We will show that much faster computations can be achieved by focusing on, for example, ignition timing alone. It is possible to remove from the detailed mechanism reactions and species that do not significantly contribute to the chemistry that leads up to the ignition event. The automatic procedure for simplifying the detailed mechanism is presented below, after a discussion of the numerical model of HCCI combustion.

HCCI ANALYSIS WITH SEQUENTIAL FLUID DYNAMICS AND CHEMISTRY

Homogeneous Charge Compression Ignition (HCCI) engines are being considered as a future alternative for diesel engines. HCCI engines have the potential for high efficiency (diesel-like [7]), very low nitrogen oxide (NOx) and particulate matter emissions, and low cost (because no high-pressure injection system is required). Disadvantages of HCCI engines are high hydrocarbon (HC) and carbon monoxide (CO) emissions, high peak pressures, high rates of heat release, reduced engine speed range, reduced power per displacement, and difficulty in starting and controlling the engine.

It is generally accepted that HCCI combustion is dominated by chemical kinetics [8], with no requirement for flame propagation. This notion has been supported by spectroscopy experiments, which indicate that the order of radical formation in HCCI combustion corresponds to self-ignition instead of flame propagation [9,10]. If a truly homogeneous mixture exists at the time of combustion, turbulence has little direct effect on HCCI combustion, but it may have an indirect effect by altering the temperature distribution and the boundary layer thickness within the cylinder. Small temperature differences inside the cylinder have a considerable effect on combustion because chemical kinetics is very sensitive to temperature.

Turbulence introduces great complexity to the analysis of spark-ignited and compression-ignited engines. The fact that HCCI combustion is not very sensitive to turbulence opens the possibility of developing a thorough, accurate

method of simulation of HCCI combustion. In principle, a comprehensive model of engine combustion would be obtained by combining a computational fluid dynamics (CFD) code and a detailed chemical kinetics code. In this approach, the CFD code would calculate the temperature and composition distribution within the cylinder while simultaneously the chemical kinetics code would calculate chemical heat release as a function of pressure, temperature and composition; in each cell. The simultaneous calculation of a detailed fluid mechanics code with a detailed chemical kinetics code is well beyond our current computational capabilities. Considering that even a two-dimensional spatial grid requires thousands of CFD elements to obtain a good definition of the boundary layer and crevices, solving the simultaneous fluid flow with chemical kinetics problem would imply having to solve for thousands of well-stirred reactors, interacting with one another through heat transfer, diffusion, convection, and compression work. This is an intractable task for current computers, even when the simplest fuels (e.g., hydrogen, methanol) are considered.

Instead of attempting the overwhelmingly long task of simultaneous numerical solution of fluid mechanics and chemical kinetics, we have developed an alternative, sequential procedure for simulation of HCCI combustion [11-13]. The procedure uses a two-step approach. First, a fluid mechanics code (KIVA3V [14]) is used to calculate temperature histories during the compression stroke. The engine geometry-specific information calculated by KIVA3V is then handed off to a detailed chemical kinetics code (HCT; Hydrodynamics, Chemistry and Transport [15]). HCT models the combustion chamber as several fixed mass reactors (called zones) that have temperatures as determined from the KIVA3V code.

We have found that a small number of HCT zones (10) is enough to obtain accurate results; this is the big advantage of this sequential KIVA3V-HCT procedure. This procedure achieves the benefits of linking the fluid mechanics (KIVA3V) and the chemical kinetics (HCT) with a great reduction in the computational effort. Thus, an HCCI simulation can be handled with current computers. The methodology also shows promise for generating quantitative predictions for HC and CO emissions, and it is capable of predicting where in the cylinder the different pollutants are being generated. In addition to this, this method offers insight into the detailed chemical kinetics of the HCCI combustion process.

The advantages of the sequential KIVA3V-HCT procedure compared to simultaneous computations are qualitatively illustrated by Figures 1 and 2. Figure 1 shows that current computers can solve the problem of detailed fluid mechanics with very simplified chemistry, or the problem of detailed chemical kinetics with very simplified fluid mechanics. The problem of detailed fluid mechanics linked with detailed chemistry is well beyond the capabilities of even the fastest computers, making it impossible to obtain accurate predictions for spark-

ignited and diesel engines. However, for HCCI combustion, the fluid mechanics and the chemistry are very much uncoupled. It is therefore possible to obtain a solution to the detailed fluid mechanics problem and a solution to the detailed chemical kinetics problem. These solutions can then be combined to obtain a solution for HCCI combustion that is much closer to the solution of the real problem than could otherwise be achieved with current computers (Figure 2).
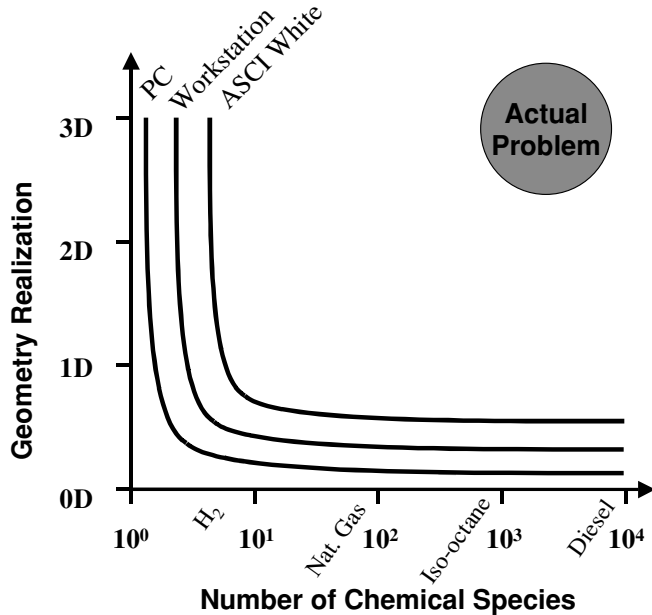

Figure 1. Qualitative representation of the capabilities of current computers, including a PC, a workstation and the fastest DOE (US Department of Energy) computer (ASCI White).

The sequential KIVA3V-HCT methodology has been successfully applied to HCCI engines running on natural gas [11], propane [12] and iso-octane [13]. While the procedure has general applicability to any fuel, computational time grows quickly as the number of zones and the number of species in the chemical kinetic mechanism is increased. Computational time is linearly proportional to the number of zones and proportional to the square of the number of species [13]. The running time for a 10-zone problem with propane is about 2 hours, and for the full iso-octane mechanism it is of the order of 2 days. Thus, even with the computational time savings of the sequential KIVA3V-HCT methodology for HCCI simulation, the computational time is far too long to practically perform sensitivity and optimization studies. It is clearly desirable to reduce the running time.

REDUCED CHEMICAL MECHANISM AUTOMATICALLY GENERATED BY COMPUTER

The reduced mechanism is developed from the detailed mechanism by eliminating unimportant reaction steps and species. We can not tell in advance what reactions and species are unimportant. We first solve the problem,

or a closely related problem, using the detailed chemical kinetic mechanism to create a single "detailed solution." From examination of the "detailed solution," we can, in retrospect, decide which reactions and species may be removed. In the case of HCCI ignition, we find that an adequate "detailed solution" is generated by simply modeling HCCI as a single zone; i.e. as a well-stirred reactor with a compression and expansion stroke; we stop the computation upon ignition. It is from this "detailed solution" that we generate the reduced mechanism.
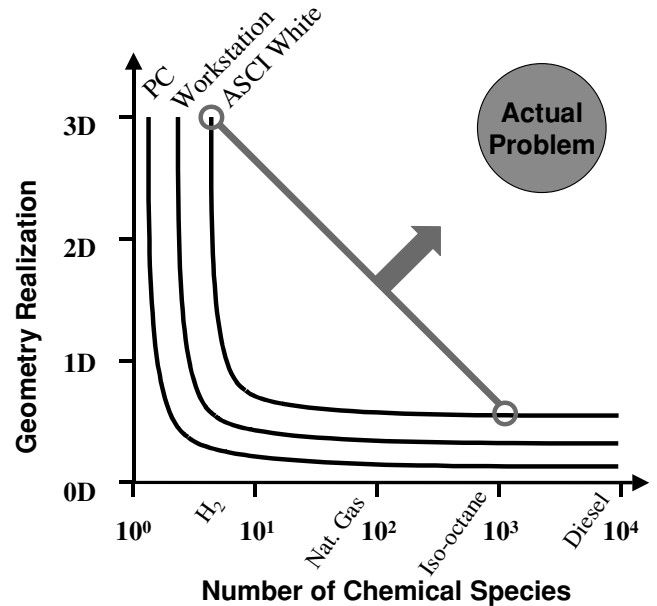
Figure 2. Qualitative representation of the capabilities of current computers, including a PC, a workstation and the fastest DOE computer (ASCI White). For HCCI combustion it is possible to obtain solutions to a detailed fluid mechanics problem and to a detailed chemical kinetics problem, and combine them to obtain a solution that is very close to the solution to the real problem.

The strategy for identifying the unimportant reaction steps is to examine their normalized first-order sensitivity coefficients defined in the customary way from the reaction rates; in practice, it suffices to use the A-factor alone:

$$\left(\frac{\partial \ln X_k}{\partial \ln \alpha_i}\right) \Big/ \max_i \left|\frac{\partial \ln X_k}{\partial \ln \alpha_i}\right| \text{ or } \left(\frac{\partial \ln T}{\partial \ln \alpha_i}\right) \Big/ \max_i \left|\frac{\partial \ln T}{\partial \ln \alpha_i}\right|,$$

where α_i is the "A-factor" in the Arrhenius expression for the forward rate constant, $k_f = \alpha T^{\beta} \exp(\frac{-E_A}{RT})$,

and X_k is the mole fraction of the k-th species. A reduced mechanism consists of only those reaction steps having normalized sensitivity coefficients greater than a certain level, e.g., usually a 5% cut-off level.

In addition we examine the normalized production or destruction rates and their definitions are given as:

Normalized production value

$$\overline{C}_{ki}^p = \frac{\max(\nu_{ki},0)q_i}{\sum_{i=1}^{I}\max(\nu_{ki},0)q_i}$$

Normalized destruction value

$$\overline{C}_{ki}^d = \frac{\min(\nu_{ki},0)q_i}{\sum_{i=1}^{I}\min(\nu_{ki},0)q_i},$$

where ν_{ki} is the stoichiometric coefficient of k-th species in i-th reaction, q_i is the rate of reaction progress variable for the i-th reaction step, and I is the total number of reaction steps. It is possible that the first-order sensitivity coefficient of a species with respect to a certain reaction step is small although the corresponding normalized production or destruction value of that species is large. This particular reaction step would be eliminated by using the sensitivity analysis only; but in fact must be included into the reduced mechanism.

Based on the above considerations, a procedure has been established to construct the reduced mechanism:

We initially include those species with concentrations greater than a preset threshold, say $1.x10^{-5}$ mole fraction (this is 10 parts per million (ppm)). Additional species may be picked up in step (4) and the final reduced mechanism is not sensitive to the threshold choice [16].

For each species, select reaction rates with sensitivity coefficients $(\frac{\partial \ln X_k}{\partial \ln \alpha_i})\Big/\max_i\left|\frac{\partial \ln X_k}{\partial \ln \alpha_i}\right|$ larger than a certain level, e.g., usually a 5% cut-off level. This set of reaction rates forms the first iteration to the reduced mechanism.

There may be reactions remaining in the detailed mechanism that contribute significantly to production (or destruction) of a species that is in the reduced mechanism. If so, we must add these reactions to the reduced mechanism. Thus, we examine the reaction steps that are not in the reduced mechanism to see if values of $\overline{C}_{ki}^p$ or $\overline{C}_{ki}^d$ for the species, that are in the reduced mechanism, are larger than a certain threshold, e.g., usually a 5%. If so, those reactions will be added to the preliminary set.

Now that we have added more reactions to the reduced mechanism, we check if we have also added new species, from the detailed mechanism to the reduced mechanism. If yes, we then go to step (2) above and iterate again. In practice no more than 10 iterations have been needed.

In theory, a reduced mechanism should be generated from each time step of the detailed solution; fortunately, in practice, a satisfactory reduced mechanism can be generated from several judiciously chosen time steps.

We used the above algorithm to generate a reduced mechanism for application to HCCI engines running under wide ranges of conditions. These are listed in Table 1. The resulting reduced mechanism contains 199 species and 383 reactions, while the original detailed mechanism [17] contains 859 species and 3606 reactions. We note in passing, that these matrices $\overline{C}_{ki}^p$ or $\overline{C}_{ki}^d$ are uncommonly large, being the dimension of 859 times 3606; (roughly 50 megabytes of double precision).

Table 1. List of conditions for generation of the reduced mechanism.

Parameter	Minimum value	Maximum value
Pressure	1 bar	3 bar
Temperature	353 K	423 K
Residual gas fraction	0	0.7
Equivalence ratio	0.2	0.6
Compression ratio	10	18

The applicability of a reduced mechanism is increasingly suspect when the reduced mechanism is used to solve a problem that is increasingly outside the bounds of the problem that was used for the reduction.

RESULTS

The detailed mechanism and the reduced mechanism have been applied to analyze two cases of HCCI combustion of iso-octane. The experiments were conducted on a Cummins C engine with a bowl-in-piston geometry. The characteristics of the engine are listed in

Table 2, and the operating conditions for the two cases being analyzed are listed in Table 3. The analysis methodology is described in detail in previous publications [11-13].

Table 2. Main characteristics of the Cummins C single cylinder engine used for the HCCI experiments.

Displaced volume	1378 cm^3
Bore	114 mm
Stroke	135 mm
Connecting rod length	216 mm
Geometric compression ratio	10.5:1
Exhaust valve open	135° ATDC
Exhaust valve close	370° ATDC
Intake valve open	350° ATDC
Intake valve close	574° ATDC
Geometry	Cylindrical bowl-in-piston

Table 3. Main HCCI combustion characteristics of the two cases selected for analysis.

	Case 1	Case 2
Engine speed, rpm	1010	2007
Intake temperature, K	381	413
Absolute intake pressure, bar	2.41	3.11
Equivalence ratio	0.346	0.348
Swirl ratio	3.6	3.6
Peak cylinder pressure, bar	109.3	112.4
CAD for peak heat release	0.5 ATDC	7.0 ATDC
burn duration, CAD[1]	6.3	9.6
Combustion efficiency, %	96.1	96.1
Gross IMEP, bar	9.4	10.7
Coefficient of variation in gross IMEP, %	2.3	3.2
Gross indicated efficiency, %	40.5	43.4
HC emissions, g/kg fuel	34.2	32.0
CO emissions, g/kg fuel	21.7	31.5
NO_x emissions, g/kg fuel	0.228	0.228
NO_x emissions, ppm	5.25	5.28

1. Burn duration is defined as the crank angle between the two points at which apparent heat release is 10% of the peak heat release.

Figure 3 shows a comparison between experimental pressure traces and numerical pressure traces for the two cases being considered. Two numerical pressure traces are included for each experimental pressure trace, corresponding to the detailed chemical kinetic mechanism and the reduced mechanism. Figure 3 shows an excellent agreement between experimental and numerical pressure traces for Cases 1 and 2. The agreement holds during the compression stroke as well as during the expansion stroke. Figure 3 shows that both the reduced and the detailed mechanisms yield results that follow very closely the experimental results.
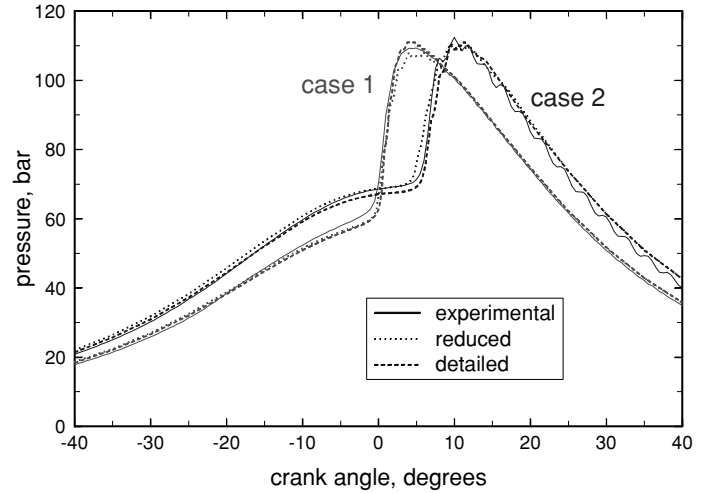

Figure 3. Comparison between experimental pressure traces and numerical pressure traces for the two cases being considered. Two numerical pressure traces are included for each experimental pressure trace, corresponding to the detailed chemical kinetic mechanism and the reduced mechanism.

Figure 4 shows a comparison between experimental and numerical apparent heat release rates. Once again, the figure shows two numerical heat release rates for each experimental heat release rate, corresponding to the detailed and the reduced chemical kinetic mechanisms. The figure shows that the reduced mechanism produces better predictions for heat release rates than the detailed mechanism. The reduced mechanism predicts very well the peak heat release as well as the width of the experimental heat release, especially for Case 2. The detailed mechanism tends to overpredict the maximum heat release rates, especially for Case 1. This better agreement by the reduced chemistry is fortuitous as the performance of reduced chemistry at best matches those of detailed chemistry. The numerical results presented in Figure 4 are considered to be in excellent agreement with the experimental results. Heat release rate is typically difficult to match numerically because heat release rate is obtained by analyzing the derivative of the pressure traces (data) applying to the first law of thermodynamics [18]. Small inaccuracies (noise) in pressure data are amplified by the derivative and can therefore result in great differences in apparent heat release rates.

Figure 5 shows a comparison between experimental and numerical results for the main combustion parameters of HCCI, for the two cases being analyzed. Again, the

figure shows two numerical results for each experimental result, corresponding to the reduced and the detailed chemical kinetic mechanisms. The figure shows that the results for peak cylinder pressure, indicated efficiency and combustion efficiency match very closely the experimental results (listed in Table 3). The maximum difference for these parameters is 3% for the combustion efficiency, and the average error is significantly lower than that (1%). Burn duration (defined as the crank angle between the two points at which apparent heat release is 10% of the peak heat release) is underpredicted by about 10% for the detailed mechanism. The reduced mechanism can predict the burn duration with better accuracy.
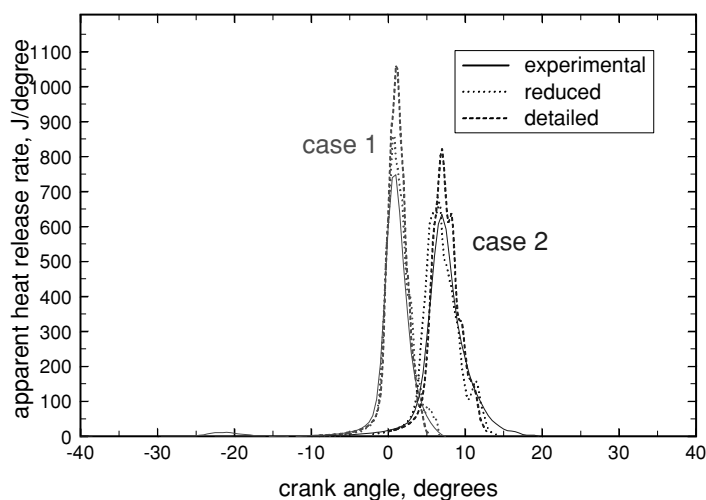

Figure 4. Comparison between experimental and numerical apparent heat release rates. The figure shows two numerical heat release rates for each experimental heat release rate, corresponding to the detailed and the reduced chemical kinetic mechanisms.

also plays an important role in predicting CO emissions. Ten zones are typically not enough to accurately resolve the field to yield precise CO emission predictions [19]. CO emissions originate within a very narrow temperature range. Typically 40 zones are necessary to make sure that this narrow temperature range is properly resolved. As the chemistry for CO in the low-temperature crevices is different from those controlling ignition, a different reduced chemistry may be necessary for better predictions of CO and hydrocarbon emissions. One possibility is to run a well-mixed reactor for a misfire case and use it for developing a reduced chemistry for partial oxidation of isooctane into CO and hydrocarbons.
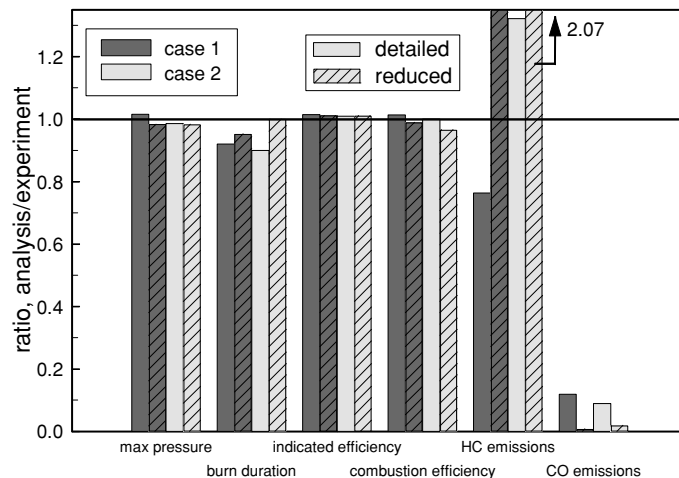

Figure 5. Comparison between experimental and numerical results for the main combustion parameters of HCCI, for the two cases being analyzed. The figure shows two numerical results for each experimental result, corresponding to the reduced and the detailed chemical kinetic mechanisms.

Not surprisingly, the detailed mechanism predicts hydrocarbon and carbon monoxide emissions better than the reduced mechanism. The reduced mechanism overpredicts hydrocarbon emissions by a factor of 1.35 in Case 1 and by a factor of 2 in Case 2. The detailed mechanism predicts 75% and 130% of the experimental hydrocarbon emissions respectively for Cases 1 and 2. CO emissions are greatly underestimated in all cases. The detailed mechanism predicts about 10% of the experimental CO emissions. The reduced mechanism predicts almost 2 orders of magnitude less CO than measured experimentally. This is due to the fact that the reduced mechanism was targeted to predict HCCI ignition and not to predict CO emissions. In addition to this, CO emissions are intrinsically difficult to predict. During combustion, CO is an intermediate combustion product. Fuel is first converted into intermediate hydrocarbons, which then react to form CO. Carbon monoxide finally reacts with OH to generate CO_2 after all the hydrocarbons are consumed (OH reacts with hydrocarbons much faster than with CO). Resolution

CONCLUSION

A reduced chemical kinetics mechanism for iso-octane has been derived from a detailed mechanism by eliminating unimportant reaction steps and species. The reduced mechanism has been developed for conditions typical of HCCI combustion. The reduced mechanism contains 199 species and 383 reactions, while the original detailed mechanism contains 859 species and 3606 reactions.

The reduced mechanism has been applied to a multi-zone analysis of iso-octane HCCI combustion by using a sequential methodology previously demonstrated by the authors. The multi-zone analysis takes into account the temperature distribution that exists inside the combustion chamber and has been used in the past to obtain accurate predictions of HCCI combustion and emissions. The main conclusions of this work are as follows.

The reduced chemical kinetic mechanism does an excellent job predicting pressure traces and heat release rates. Pressure traces and heat release rates obtained with the reduced mechanism are comparable to (and in some cases better than) the results obtained with the detailed mechanism.

The detailed mechanism generates better predictions for HCCI emissions than the reduced mechanism. The reduced mechanism considerably overpredicts hydrocarbon emissions (by as much as a factor of 2 in one case). Carbon monoxide is underpredicted in all cases. The detailed mechanism underpredicts CO emissions by an order of magnitude, while the reduced mechanism underpredicts CO emissions by as much as 2 orders of magnitude. It is considered that this underprediction occurs because the reduced mechanism was targeted for predicting HCCI ignition, and not CO emissions. In addition to this, previous work by the authors has shown that CO emissions are intrinsically difficult to predict.

The reduced mechanism yields accurate results for HCCI combustion while reducing by a factor of 20 the computational time required to run a 10-zone problem with iso-octane fuel. The reduced model is therefore a very useful tool for sensitivity studies and optimization analyses that require multiple executions of the code.

NOMENCLATURE

$\overline{C}_{ki}^{P}$ = normalized production rate of k-th species in i-th reaction step;

$\overline{C}_{ki}^{d}$ = normalized destruction rate of k-th species in i-th reaction step;

I= total number of reaction steps;

q_i= rate of progress variable for i-th reaction step;

T= temperature;

X_k= mole fraction of k-th species;

α, α_i= A-factor in Arrhenius expression of i-th reaction step;

β, β_i= temperature exponent in Arrhenius expression of i-th reaction step;

ν_{ki}= stoichiometric coefficient of k-th species in i-th reaction step;

ACKNOWLEDGMENTS

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